

```
ring nodes :
   1 2 3 4 5 6 7 8.9
                              12 13 14 15 16 17 24 25 26 27 28
                                                                         29
                                                                              30 31
chain bonds :
   7-13 12-41 12-42 14-37 14-38 15-35 15-36 16-18 17-39 17-40 18-19 32-34
ring bonds :
   1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-9 7-8 8-9 12-13 12-17 13-14 14-15 15-16 16-17
   24-25 24-29 25-26 26-27 27-28 27-30 28-29 28-33 30-31 31-32 32-33
exact/norm bonds :
   4-7 \quad 5-9 \quad 7-8 \quad 7-13 \quad 8-9 \quad 12-13 \quad 12-17 \quad 12-41 \quad 12-42 \quad 13-14 \quad 14-15 \quad 14-37 \quad 14-38 \quad 15-16
   15-35 15-36 16-17 16-18 17-39 17-40 18-19 27-30 28-33 30-31 31-32 32-33 32-34
normalized bonds :
   1-2 1-6 2-3 3-4 4-5 5-6 24-25 24-29 25-26 26-27 27-28 28-29
isolated ring systems :
   containing 12 :
```

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS 24:Atom 25:Atom 26:CLASS 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:CLASS 35:CLASS 36:CLASS

18 19 34 35 36 37

G1:C,O,S,N

G2:C,N

G3:C,O,N

G4:H,CH3

Match level :

38

37:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS

39 40 41 42

=> d que stat

L5 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s 15

SAMPLE SEARCH INITIATED 18:03:53 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 302 TO ITERATE

100.0% PROCESSED 302 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 4998 TO 7082 PROJECTED ANSWERS: 0 TO 0

L6 0 SEA SSS SAM L5

=>

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Documents\Stnexp\Queries\10660908-3.str

chain nodes :

18 19 34 35 36 37 38 39 40 41 42

ring nodes :

1 2 3 4 5 6 7 8 9 12 13 14 15 16 17 24 25 26 27 28 29 30 31 32 33

chain bonds :

7-13 12-41 12-42 14-37 14-38 15-35 15-36 16-18 17-39 17-40 18-19 32-34 ring bonds:

exact/norm bonds :

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 24-25 24-29 25-26 26-27 27-28 28-29

isolated ring systems :

containing 12:

G1:C,O,S,N

G2:C,N

G3:C,O,N

G4:H,CH3

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS 24:Atom 25:Atom 26:CLASS 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:CLASS 35:CLASS 36:CLASS 37:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS

L7 STRUCTURE UPLOADED

=> s 17

SAMPLE SEARCH INITIATED 18:05:15 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 138 TO ITERATE

100.0% PROCESSED 138 ITERATIONS 10 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE** BATCH **COMPLETE** PROJECTED ITERATIONS: 2056 TO 3464 PROJECTED ANSWERS: 11 TO 389

L8 10 SEA SSS SAM L7

=> s 17 sss full

FULL SEARCH INITIATED 18:05:22 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 2961 TO ITERATE

100.0% PROCESSED 2961 ITERATIONS 259 ANSWERS

SEARCH TIME: 00.00.01

L9 259 SEA SSS FUL L7

=> file caplus

COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
165.63
533.85

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE
ENTRY
SESSION
CA SUBSCRIBER PRICE

0.00 -29.20

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FILE COVERS 1907 - 18 Sep 2005 VOL 143 ISS 13 FILE LAST UPDATED: 16 Sep 2005 (20050916/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 19 L10 8 L9

=> d l10 1-8 bib abs fhitstr

L10 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2005:638875 CAPLUS

DN 143:153404

TI Preparation of N-substituted piperidine and piperazine derivatives dopamine D2 and serotonin 2A receptor antagonists

- IN Cho, Stephen Sung Yong; Gregory, Tracy Fay; Guzzo, Peter Robert; Howard, Harry Ralph, Jr.; Nikam, Sham Shridhar; Surman, Matthew David; Walters, Michael Anthony
- PA Warner-Lambert Company Llc., USA
- SO PCT Int. Appl., 144 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN. CNT 1

rAN.	CNT	т																
	PA?	CENT 1	NO.			KIND DATE		APPLICATION NO.						DATE				
PΙ	WO	WO 2005066165		A1		2005	0721	1	WO 2	004-	IB42	39		20041220				
		W:	ΑE,	AG,	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
			CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
			GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KP,	KR,	ΚZ,	LC,
			LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NI,
			NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,
			ТJ,	TM,	TN,	TR,	TT,	TZ,	UA,	ŪG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW
		RW:	BW,	GH,	GM,	KE,	LS,	MW,	ΜZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,
			ΑZ,	BY,	KG,	ΚZ,	MD,	RU,	ТJ,	TM,	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,
			EE,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,	IS,	IT,	LT,	LU,	MC,	NL,	PL,	PT,
			RO,	SE,	SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,
			MR,	NE,	SN,	TD,	TG											
PRAI	PRAI US 2003-533761P							2003	1231									

PRAI US 2003-533761P P 20031231

AΒ This invention relates to N-substituted piperidine and piperazine derivs. (shown as I; variables defined below; e.g. [5-[2-[4-(benzo[d]isothiazol-3yl)piperazin-1-yl]ethyl]-3,3-dimethyl-2,3-dihydroindol-1-yl](4fluorophenyl)methanone (shown as II)), pharmaceutical compns. contg. them and their use in the treatment of central nervous system and other disorders. Although the methods of prepn. are not claimed, example prepns. and/or characterization data for .apprx.160 I are included. For example, II was prepd. in 98 % yield by coupling 3-[4-[2-(3,3-dimethyl-2,3dihydro-1H-indol-5-yl)ethyl]piperazin-1-yl]benzo[d]isothiazole with 4-fluorobenzoyl chloride; the benzo[d]isothiazole reactant was prepd. in 79 % yield by redn. of 5-[2-[4-(benzo[d]isothiazol-3-yl)piperazin-1yl]ethyl]-3,3-dimethyl-1,3-dihydroindol-2-one, which was prepd. in 96 % yield from 3-(piperazin-1-yl)benzo[d]isothiazole and 5-(2-chloroethyl)-3,3dimethyl-1,3-dihydroindol-2-one, which was prepd. in 45 % yield by redn. of 5-(2-chloroethyl)-3,3-dimethyl-1,3-dihydroindol-2-one, which was prepd. in >96 % yield from chloroacetyl chloride and 3,3-dimethyl-1,3dihydroindol-2-one. For I: M = E-R9, L-T-R9, T-D-R9; U is S, O, SO, SO2, CH2 or NR3; V is N or C; Z is N or C; A is -(CH2)mO-, -(CH2)mNR4-, or -(CH2)mC(R5R6)-, wherein R5 and R6 = H, (C1-C4) alkyl (un) substituted with 1-3 F atoms, (C1-C4) alkoxy (un) substituted with 1-3 F atoms, hydroxy, and aminoalkyl; or R5 and R6 together form a carbonyl, and wherein m = 1-4. R1 and R2 = H, (C1-C4) alkyl (un)substituted with 1-3 F atoms, (C1-4) alkoxy (un) substituted with 1-3 F atoms, halogen, nitro, cyano, amino, (C1-C4) alkylamino and di(C1-C4) alkylamino; R3 and R4 = H, (C1-C4) alkyl (un) substituted with 1-3 F atoms and (C1-C4) alkoxy (un) substituted with 1-3 F atoms; or, when U is NR3, one of R1 and R2 can form, together with the C to which it is attached, and together with R3 and the N to which it is attached, a heterocyclic ring contg. 4-7 ring members of which 1-3 ring members can be N, O and S, and of which the remaining ring members are C, with the proviso that when R3 forms a ring with one of R1 and R2, the other of R1 and R2 is absent. X is -[C(R11)(R12)]o-, wherein R11 and R12 = H and (C1-C4) alkyl (un)substituted with 1-3 F atoms, and wherein o = 0-3, with the proviso that when W is absent, o .qtoreq.2; W is -[C(R13)(R14)]p-, wherein R13 and R14 = H and (C1-C4) alkyl (un) substituted with 1-3 F atoms, and wherein p = 0-4, with the proviso that when X is absent, p .gtoreq.2; R7 and R8 = halo, R1 and -OR1; or R7, when attached to a C adjacent to one of the C atoms shared by both the Ph

ring to which R7 is attached and the ring contg. W, N and X, forms, together with a C atom of X or a C atom of W, a satd. carbocyclic ring contg. 3-6 C atoms. R9 = Ph, phenoxy, benzyloxy, and phenylamino, wherein the Ph moieties are (un) substituted with 1-3 halo, (C1-C3) alkyl (un) substituted with 1-3 F atoms, (C1-C3) alkoxy (un) substituted with 1-3 F atoms, nitro, cyano, amino, and (C1-C3) alkylamino; or R9 is a pyrrolidine, piperidine or morpholine ring wherein the point of attachment to D, T or E is the ring N, and wherein said pyrrolidine, piperidine or morpholine ring can be (un) substituted with 1 or 2 Me, amino, (C1-04) alkylamino, and di(C1-C4) alkylamino; or R9 is a furan, thiophene, or pyrazole ring (un) substituted with 1-2 (C1-C4) alkyl groups; or R9 is (C1-C6) straight or branched alkyl or (C3-C6) cycloalkyl, wherein said straight, branched and cyclic alkyl moieties are be (un)substituted with 1-3 halo atoms or (C1-C4) alkoxy (un) substituted with 1-3 F atoms; or R9 is halogen, nitro, cyano, amino, (C1-C4) alkylamino, di(C1-C4) alkylamino or OR1, wherein the alkyl moieties of (C1-C4) alkylamino and di(C1-C4) alkylamino are (un)substituted with an amino, (C1-C4) alkylamino, or di(C1-C4) alkylamino group; E is -C(0)-, -S(0)- or -SO2-; T is -C(0)- or -CO2-; L is -(CH2)n wherein n = 0-3; D is -(CHR10)q-, wherein q = 1-3, or NR10; R10 is H or straight or branched (C1-C3) alkyl.

IT 676116-01-1P, 6-[2-[4-(Benzo[d]isothiazol-3-yl)piperazin-1yl]ethyl]-4,4,8-trimethyl-3,4-dihydro-1H-quinolin-2-one
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(prepn. of N-substituted piperidine and piperazine derivs. dopamine D2 and serotonin 2A receptor antagonists)

RN 676116-01-1 CAPLUS

CN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]-3,4-dihydro-4,4,8-trimethyl- (9CI) (CA INDEX NAME)

RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:287843 CAPLUS

DN 140:321381

TI Preparation of heterocyclic substituted piperazines for the treatment of schizophrenia

IN Davis, Jamie Marie; Gregory, Tracy Fay; Walters, Michael Anthony

PA Warner-Lambert Company Llc, USA

SO PCT Int. Appl., 90 pp. CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
		-			
ΡI	WO 2004029048	A1	20040408	WO 2003-IB4113	20030918

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             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
              GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
              LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
              PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT,
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     CA 2500115
                                  20040408
                                             CA 2003-2500115
                            AA
                                                                        20030918
     EP 1546145
                            A1
                                  20050629
                                               EP 2003-798314
                                                                        20030918
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     BR 2003014796
                           Α
                                  20050726
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                                                                        20030918
                                               US 2003-672949
     US 2004067960
                            A1
                                  20040408
                                                                        20030926
PRAI US 2002-413839P
                            Ρ
                                  20020926
     WO 2003-IB4113
                            W
                                  20030918
OS
     MARPAT 140:321381
GΙ
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$$Ar-Y$$
 $N-A$
 R^2

AB The title compds. [I; Ar = 1,2-benzisothiazoyl, 1,2-benzisothiazoyl -1-oxide, naphthyl, pyridyl, etc.; with the proviso that Ar can not be attached to the piperazine ring via a Ph ring of Ar; Y = N, CH; A = (CH2)nCH2 (wherein n = 1-4, one of the CH2 groups that is not adjacent to the piperazine nitrogen can be replaced by an oxygen atom); R2, R3 = H, alkyl, fluoroalkyl, alkoxy, etc.; Q = (un)satd. (un)substituted 5-7 membered monocyclic heterocyclic ring contq. 1-3 heteroatoms selected from O, N and S], useful in the treatment of central nervous system disorders, were prepd. Thus, reacting 3-methylbut-2-enoic acid (2-{2-[4-(1,2benzisothiazol-3-yl)-piperazin-1-yl]ethyl}phenyl)amide (prepn. given) with AlCl3 in C6H5Cl afforded 8-{2-[4-(1,2-benzisothiazol-3-yl)piperazin-1yl]ethyl}-4,4-dimethyl-3,4-dihydro-1H-quinolin-2-one which showed Ki of .ltoreq. 1 .mu.M against dopamine D2 receptor binding, and Ki of .ltoreq. 1 .mu.M against 5-HT2A receptor binding. The pharmaceutical compn. comprising the compd. I is claimed.

Ι

IT 677708-34-8P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(prepn. of heterocyclic substituted piperazines for the treatment of schizophrenia)

RN 677708-34-8 CAPLUS

CN 2(1H)-Quinolinone, 8-{2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]-3,4-dihydro-4,4-dimethyl-, hydrochloride (9CI) (CA INDEX NAME)

●x HCl

RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:267327 CAPLUS

DN 140:287412

TI Preparation of piperazines as dopamine D2 and serotonin 5HT2A receptors inhibitors for the treatment of central nervous system disorders, in particular schizophrenia

IN Andreana, Tonja Lynn; Cho, Stephen Sung Yong; Graham, James Michael; Gregory, Tracy Fay; Howard, Harry Ralph, Jr.; Kornberg, Brian Edward; Nikam, Sham Shridhar; Pflum, Derek Andrew

PA Warner-Lambert Company LLC, USA

SO PCT Int. Appl., 158 pp. CODEN: PIXXD2

DT Patent

LA English

FAN. CNT 1

rAN.																			
	PAT	CENT I	иО.			KIND DATE			APPLICATION NO.						DATE				
PI	WO	WO 2004026864				A1	_	2004	0401							20030905			
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			LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NI,	NO,	NZ,	OM,	
			PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	ТJ,	TM,	TN,	TR,	TT,	
			TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	zw						
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			KG,	ΚZ,	MD,	RU,	ТJ,	TM,	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	
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			BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG	
	CA	CA 2499326				AA		2004	0401	(CA 2	003-		2	0030	905			
	EP	1546	143			A1		2005	0629		EP 2	003-	7974	33		20030905			
		R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,	
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	BR	2003	0143	93		A 20050719 BR 2003-14393							20030905						
	US	US 2004138230				A1		2004	0715	US 2003-660908						20030912			

PRAI US 2002-411475P Ρ 20020917 US 2002-416355P Ρ 20021004 WO 2003-IB3902 W 20030905 os MARPAT 140:287412 GT

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [wherein X = S, O, SO, SO2, CH2, NH and derivs.; Y, Z =independently N or CH; A = (CH2)mCH2, (CH2)mO, (CH2)mNR9, (CH2)mC(R7R8); R7, R8 = independently (un)substituted alkyl, alkoxy, or CR7R8 = carbonyl; m = 1-4; R4, R5 = independently H, (un) substituted alkyl, alkoxy, or when X = NR6 and derivs., CR4R5R6N = 4-7 membered heterocyclyl ring, with the proviso that when R9R4 or R9R5 = a ring, the other of R4 and R5 is absent; R9 = H, (un)substituted alkyl, alkoxy; R6 = H, (un)substituted alkyl, alkoxy; R1 = H, (un)substituted alkyl; R2, R3 = independently H, halo, hetero/aryl, (un)substituted aryl/heteroarylalkyl, alkoxy, etc.; V, W = independently CH2 and derivs. or CH and derivs.; and their pharmaceutically acceptable salts] were prepd. s dopamine D2 and serotonin 5HT2A receptors inhibitors for treating central nervous system disorders, in particular schizophrenia (no data). For example, II.bul.MeSO3H was prepd. by acylation of 3-chloro-2-methylaniline with 3,3-diethylacryloyl chloride, one-pot Friedel-Craft alkylation with chloroacetyl chloride and cyclization in the presence of AlCl3 to chloroacetylquinoline intermediate, redn. to chloroethylquinoline III, alkylation of 3-(piperazin-1-yl)benzo[d]isothiazole hydrochloride with III, followed by salt formation of II with methanesulfonic acid. II acted as dopamine D2 and serotonin 5HT2A receptors inhibitors with a Ki value of 0.9 nm and 1 nM, resp. Thus, I and their formulations are useful for treating central nervous system disorders, in particular schizophrenia and depression. 676117-35-4P, 2-[6-[2-[4-(Benzo[d]isothiazol-3-yl)piperazin-1-IT yl]ethyl]-3-methyl-2-oxo-3,4-dihydro-2H-quinolin-1-yl]acetamide RL: CPN (Combinatorial preparation); PAC (Pharmacological activity); THU

(Therapeutic use); BIOL (Biological study); CMBI (Combinatorial study); PREP (Preparation); USES (Uses)

(drug candidate; prepn. of piperazines for treating of central nervous system disorders, in particular schizophrenia)

RN 676117-35-4 CAPLUS

1(2H)-Quinolineacetamide, 6-[2-[4-(1,2-benzisothiazol-3-y1)-1piperazinyl]ethyl]-3,4-dihydro-3-methyl-2-oxo- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & &$$

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD

ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2002:732486 CAPLUS

DN 138:331185

TI New 3-benzisothiazolyl and 3-benzisoxazolylpiperazine derivatives with atypical antipsychotic binding profile

AU Orjales, Aurelio; Mosquera, Ramon; Toledo, Antonio; Pumar, Carmen; Labeaga, Luis; Innerarity, Ana

CS Research Department, FAES FARMA, S.A., Leioa, E-48940, Spain

SO European Journal of Medicinal Chemistry (2002), 37(9), 721-730 CODEN: EJMCA5; ISSN: 0223-5234

PB Editions Scientifiques et Medicales Elsevier

DT Journal

LA English

OS CASREACT 138:331185

AB New 3-benzisothiazolyl and 3-benzisoxazolylpiperazine derivs. were synthesized and their 5-HT1A, 5-HT2A and D2 receptor binding affinities evaluated. The compds. displayed high affinity for the 5-HT2A receptor combined with moderate to low 5-HT1A and D2 affinities. Two of them have been selected for further pharmacol. studies to be evaluated as potential atypical antipsychotics.

IT 516509-59-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(benzisothiazolyl and benzisoxazolylpiperazine derivs. with atypical antipsychotic binding profile)

RN 516509-59-4 CAPLUS

CN 2(1H)-Quinolinone, 1-[2-[4-(1,2-benzisoxazol-3-yl)-1-piperazinyl]ethyl]-3,4-dihydro-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1999:10184 CAPLUS

DN 130:38398

10/460752

TI Quinolin-2(1H)-one derivatives as serotonin antagonists

IN McCort, Gary; Hoornaert, Christian; Duclos, Olivier; Cadilhac, Caroline; Guilpain, Eric

PA Synthelabo S. A., Fr.

SO Fr. Demande, 38 pp. CODEN: FRXXBL

DT Patent

LA French

FAN.CNT 1

t was	CNII				
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
					
PΙ	FR 2761067	A 1	19980925	FR 1997-3388	19970320
	FR 2761067	B1	19990423		
PRAI	FR 1997-3388		19970320		
os	MARPAT 130:38398				
GI					

$$O_2N$$
 O_2N
 O_2N

AB Quinolinones I [R1, R2 = H, halogen, NH2, OH, NO2, CN, alkyl, alkoxy, CF3, OCF3, CO2R5, carbamoyl, SR5, SO2R5, NHNCOR5, NHSO2R5, NR52 (R5 = alkyl); R3 = H, (un)substituted alkyl; R4 = H, halogen, OH, NO2, CN, alkyl, alkoxy, CF3, CONH2, NHSO2Me; m = 2-4; Z = N, CH; A = O, NH, S, NR5] were prepd. for use as serotonin antagonists (no data). Thus, the quinolinone II was obtained from the chloroethylquinolinone and the piperidinylisoxazole fragments.

Ι

IT 216674-97-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of quinolinone derivs. as serotonin antagonists)

RN 216674-97-4 CAPLUS

CN 2(1H)-Quinolinone, 7-fluoro-4-[2-[4-(6-fluoro-1H-indazol-3-yl)-1-piperazinyl]ethyl]- (9CI) (CA INDEX NAME)

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L10 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN
    1995:682542 CAPLUS
AN
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DN 123:83356

Preparation of 3-(1-piperazinyl)-1,2-benzisothiazole derivatives with TI antipsychotic effect

Fukuda, Yoshimasa; Sasaki, Toshiro; Nakatani, Yuuko; Ichimaru, Yasuyuki; IN Imanishi, Taiichiro

PA Meiji Seika K. K., Japan

so PCT Int. Appl., 95 pp. CODEN: PIXXD2

DT Patent

LА Japanese

FAN.	CNT 1														
	PATENT I	NO.			KINI	DATE		AP	PLICAT	ION N	ю.		D <i>I</i>	ATE	
													·		
ΡI	WO 9418	197			A 1	1994	0818	WO	1994-	JP159)		19940203		
	W:	CN,	JP,	KR,	US										
	RW:	ΑT,	BE,	CH,	DE,	DK, ES,	FR,	GB, GI	R, IE,	IT,	LU,	MC,	NL,	PT,	SE
	EP 635506					1995	0125	EP	1994-	90584	1		19940203		
	R:	AT,	BE,	CH,	DE,	DK, ES,	FR,	GB, I	r, LI,	NL,	SE				
	CN 1103	534			Α	1995	0607	CN	1994-	19004	2		19	99402	203
	CN 1050	604			В	2000	0322								
	US 5599	815			Α	1997	0204	US	1994-	31885	57		19	99412	220
PRAI	JP 1993	-1750)5		Α	1993	0204								
	WO 1994	-JP1			Α	1994	0104								
	WO 1994	-JP15	9		W	1994	0203								
os	MARPAT	123:8	335	6											
GI															

AB Compds. represented by general formula [I; n = 2-4; W = heterocycly], e.g., Q - Q2; m = 0-2; A = CH2, CH, N, NH; B = CH2, CH, N, NH, S; provided that both A and B .noteq. N or NH; X = CH, N, S, bond; Y = CH, N; R1 = H, halo, lower (halo)alkyl, (un)substituted Ph, OH, NO2, lower alkoxy, NH2, cyano; R2, R3 = H, halo, lower (halo)alkyl or alkoxy, NH2, cyano, provided that when X = bond, R2 is not present; or R2R3 = (CH2)p (wherein p = 3-5)] and pharmacol. acceptable salts thereof, reduced in the adverse effect against the extrapyramidal system and hence useful as an antipsychotic agent with few side effects, are prepd. Thus, 0.29 g 2-hydroxyquinoline was dissolved in DMF and treated with 80 mg NaH at 60.degree. for 30 min with stirring followed by cooling the reaction mixt. to room temp. and adding 2.16 g 1,4-dibromobutane and the resulting mixt. was stirred at 60.degree. for 4 h to give 64% 1-(4-bromobutyl)-2(1H)-quinolinone (II). II 0.56, 3-(1-piperazinyl)-1,2-benzisothiazole 0.44, and K2CO3 0.33 g were suspended in DMF and stirred at room temp. for 12 h to give 80% title compd. I (n = 4, W = 2-oxo-1, 2-dihydro-1-quinolinyl). II (n = 4, W = 9-carbazolyl) and II (n = 3, W = 2-oxo-1, 2-dihydro-1-quinolinyl) showedED50 of 1.15 and 0.92 mg/kg i.p., resp., for inhibiting methamphetamine-induced spontaneous movement of mice (vs. 0.16 and 1.05 mg/kg i.p. for haloperidol and chlorpromazine, resp.) and induced catalepsy in mice at ED50 of >100 and 83.3 mg/kg i.p. in mice (vs. 1.3 and 6.2 mg/kg i.p. for haloperidol and chlorpromazine, resp.).

IT 165109-31-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of [N-(heterocyclylalkyl) piperazinyl] benzisothiazole derivs. as antipsychotics)

RN 165109-31-9 CAPLUS

2(1H)-Quinolinone, 1-[4-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]butyl]-, monohydrochloride (9CI) (CA INDEX NAME)

CN

● HCl

L10 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN 1995:657604 CAPLUS DN 123:55870 TI Preparation of indazole derivatives as antipsychotics IN Sasaki, Toshiro; Nakatani, Juko; Hiranuma, Toyoichi; Kashima, Hiroko; Fukuda, Yoshimasa PA Meiji Seika Co, Japan SO Jpn. Kokai Tokkyo Koho, 23 pp. CODEN: JKXXAF DΤ Patent Japanese LА FAN.CNT 1 DATE APPLICATION NO. DATE PATENT NO. KIND ---------PI JP 07033744 A2 19950203 JP 1993-204612 19930727 PRAI JP 1993-204612 19930727 MARPAT 123:55870

OS

GI

$$V = \begin{bmatrix} N & \text{N (CH2)} & \text{NW} \\ N & \text{NM} & \text{NM} \end{bmatrix}$$

AB The title compds. I [n = 2 - 6; V = H, halo; R1 = H, alkyl, etc.; W = heterocycle (further details on said heterocycle are given)] are prepd. Indazole deriv. II (prepn. given) showed ED50 of 0.50 mg/Kg i.p. against methamphetamine-induced activities in mice, vs. ED50 of 0.16 mg/Kg i.p. shown by haloperidol. In a test for catalepsy-causing activity in mice, II showed ED50 of 18 mg/Kg i.p., vs. ED50 of 1.3 mg/Kg i.p. shown by haloperidol.

IT 164519-46-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

II

(prepn. of indazole derivs. as antipsychotics)

RN 164519-46-4 CAPLUS

CN 6(5H)-Phenanthridinone, 5-[4-[4-(1H-indazol-3-yl)-1-piperazinyl]butyl]-(9CI) (CA INDEX NAME)

L10 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1991:492295 CAPLUS

DN 115:92295

TI Preparation of heteroarylpiperazines as antipsychotic agents

IN Howard, Harry R.

PA Pfizer Inc., USA

10/460752

SO Eur. Pat. Appl., 20 pp.

CODEN: EPXXDW

DT Patent LA English FAN.CNT 1

GΙ

	O., 1					
	PATENT NO.	KIND DATE	APPLICATION NO.	DATE		
PI	EP 409435	A1 19910123	EP 1990-307166	19900629		
	EP 409435	B1 19941026				
	R: AT, BE, CH,	DE, DK, ES, FR, G	B, GR, IT, LI, LU, NL,	SE		
	WO 9100863	A1 19910124	WO 1989-US2954	19890707		
	W: FI, HU, NO,	RO, SU, US				
	ES 2062374	T3 19941216	ES 1990-307166	19900629		
	JP 03044388	A2 19910226	JP 1990-176120	19900703		
	JP 07017633	B4 19950301				
	CA 2020611	AA 19910108	CA 1990-2020611	19900706		
	US 5350747	A 19940927	US 1992-836019	19920220		
PRAI	WO 1989-US2954	A 19890707				
os	MARPAT 115:92295					

$$R^{1}N$$
 $NZCH_{2}$
 N^{1}
 N^{2}
 N^{1}
 N^{2}
 N^{1}
 N^{2}
 N^{2}
 N^{3}
 N^{1}
 N^{2}
 N^{3}
 N^{4}
 N^{1}
 N^{2}
 N^{3}
 N^{4}
 N^{1}
 N^{2}
 N^{3}
 N^{4}
 N^{4}

AB The title compds. [I; W1 = CR2R3; W2 = CR4R5; W3 = CR6R7; 1 of W1-W3 may be absent; R1 = (substituted) benzisoxazolyl, benzisothiazolyl, benzopyrazolyl; R2-R7 = H, alkyl, 2 of them may form alkylene, alkenylene; X1 = H, halo, C1-4 alkyl, alkoxy, NO2, cyano, etc.; Y1 = H, C1-4 alkyl, (substituted) Ph, etc.; X1Y1 = heterocyclyl; Z = C1-6 alkylene], useful as antipsychotic agents (no data), were prepd. A mixt. of piperazine deriv. II, quinolinone III (prepn. given), Na2CO3, and KI in MIBK was heated at 90.degree. under N to give 13% title compd. IV, sepd. as HC1.1/2 H2O. Also prepd. were 17 addnl. I and numerous intermediates.

IT 133999-10-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of, as antipsychotic agent)

RN 133999-10-7 CAPLUS

CN 2(1H)-Quinolinone, 7-chloro-3,4-dihydro-6-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]-4,4-dimethyl- (9CI) (CA INDEX NAME)

=> d 110 4-8 bib abs hitstr

L10 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2002:732486 CAPLUS

DN 138:331185

TI New 3-benzisothiazolyl and 3-benzisoxazolylpiperazine derivatives with atypical antipsychotic binding profile

AU Orjales, Aurelio; Mosquera, Ramon; Toledo, Antonio; Pumar, Carmen; Labeaga, Luis; Innerarity, Ana

CS Research Department, FAES FARMA, S.A., Leioa, E-48940, Spain

SO European Journal of Medicinal Chemistry (2002), 37(9), 721-730 CODEN: EJMCA5; ISSN: 0223-5234

PB Editions Scientifiques et Medicales Elsevier

DT Journal

LA English

OS CASREACT 138:331185

AB New 3-benzisothiazolyl and 3-benzisoxazolylpiperazine derivs. were synthesized and their 5-HT1A, 5-HT2A and D2 receptor binding affinities evaluated. The compds. displayed high affinity for the 5-HT2A receptor combined with moderate to low 5-HT1A and D2 affinities. Two of them have been selected for further pharmacol. studies to be evaluated as potential atypical antipsychotics.

IT 516509-59-4P 516509-64-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(benzisothiazolyl and benzisoxazolylpiperazine derivs. with atypical antipsychotic binding profile)

RN 516509-59-4 CAPLUS

CN 2(1H)-Quinolinone, 1-[2-[4-(1,2-benzisoxazol-3-yl)-1-piperazinyl]ethyl]-3,4-dihydro-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 516509-64-1 CAPLUS

CN 2,4(1H,3H)-Quinolinedione, 1-[2-[4-(1,2-benzisoxazol-3-yl)-1-piperazinyl]ethyl]-3,3-dimethyl- (9CI) (CA INDEX NAME)

RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1999:10184 CAPLUS

DN 130:38398

TI Quinolin-2(1H)-one derivatives as serotonin antagonists

IN McCort, Gary; Hoornaert, Christian; Duclos, Olivier; Cadilhac, Caroline; Guilpain, Eric

PA Synthelabo S. A., Fr.

SO Fr. Demande, 38 pp. CODEN: FRXXBL

DT Patent

LA French

FAN.CNT 1

PATENT NO. KIND DATE APPLICATION NO. DATE

PI FR 2761067 A1 19980925 FR 1997-3388 19970320 FR 2761067 B1 19990423 PRAI FR 1997-3388 19970320 OS MARPAT 130:38398 GI

$$R^{1}$$
 R^{2}
 R^{3}
 R^{3}
 R^{4}

$$O_2N$$
 O_2N
 O_2N

Quinolinones I [R1, R2 = H, halogen, NH2, OH, NO2, CN, alkyl, alkoxy, CF3, OCF3, CO2R5, carbamoyl, SR5, SO2R5, NHNCOR5, NHSO2R5, NR52 (R5 = alkyl); R3 = H, (un)substituted alkyl; R4 = H, halogen, OH, NO2, CN, alkyl, alkoxy, CF3, CONH2, NHSO2Me; m = 2-4; Z = N, CH; A = O, NH, S, NR5] were prepd. for use as serotonin antagonists (no data). Thus, the quinolinone II was obtained from the chloroethylquinolinone and the piperidinylisoxazole fragments.

Ι

IT 216674-97-4P 216675-04-6P 216675-07-9P 216675-23-9P 216675-46-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of quinolinone derivs. as serotonin antagonists)

RN 216674-97-4 CAPLUS

CN 2(1H)-Quinolinone, 7-fluoro-4-[2-[4-(6-fluoro-1H-indazol-3-yl)-1-piperazinyl]ethyl]- (9CI) (CA INDEX NAME)

RN 216675-04-6 CAPLUS

CN 2(1H)-Quinolinone, 7-fluoro-4-[2-[4-(6-fluoro-1-methyl-1H-indazol-3-yl)-1-piperazinyl]ethyl]- (9CI) (CA INDEX NAME)

RN 216675-07-9 CAPLUS

CN 1(2H)-Quinolineacetamide, 7-fluoro-4-[2-[4-(6-fluoro-1-methyl-1H-indazol-3-yl)-1-piperazinyl]ethyl]-2-oxo- (9CI) (CA INDEX NAME)

Page 19

RN 216675-23-9 CAPLUS

CN 2(1H)-Quinolinone, 7-fluoro-4-[2-[4-(6-fluoro-1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]- (9CI) (CA INDEX NAME)

RN 216675-46-6 CAPLUS

CN 2(1H)-Quinolinone, 7-fluoro-4-[2-[4-(5-methoxy-1,2-benzisoxazol-3-yl)-1-piperazinyl]ethyl]- (9CI) (CA INDEX NAME)

IT 216674-09-8P 216674-18-9P 216674-23-6P

216674-30-5P 216674-36-1P 216674-43-0P

216674-49-6P 216674-53-2P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of quinolinone derivs. as serotonin antagonists)

RN 216674-09-8 CAPLUS

CN 2(1H)-Quinolinone, 4-[2-[4-(1,2-benzisoxazol-3-yl)-1-piperazinyl]ethyl]-7-fluoro-, dihydrochloride (9CI) (CA INDEX NAME)

●2 HC1

RN 216674-18-9 CAPLUS

CN 2(1H)-Quinolinone, 4-[2-[4-(6-chloro-1,2-benzisoxazol-3-yl)-1-piperazinyl]ethyl]-7-fluoro-, dihydrochloride (9CI) (CA INDEX NAME)

●2 HCl

RN 216674-23-6 CAPLUS

CN 2(1H)-Quinolinone, 7-fluoro-4-[2-[4-(6-methoxy-1,2-benzisoxazol-3-yl)-1-piperazinyl]ethyl]-, dihydrochloride (9CI) (CA INDEX NAME)

●2 HCl

RN 216674-30-5 CAPLUS

CN 2(1H)-Quinolinone, 7-fluoro-4-[2-[4-(5-methoxy-1,2-benzisoxazol-3-yl)-1-piperazinyl]ethyl]-, dihydrochloride (9CI) (CA INDEX NAME)

●2 HCl

RN 216674-36-1 CAPLUS

CN 2(1H)-Quinolinone, 7-fluoro-4-[2-[4-(6-fluoro-1H-indazol-3-yl)-1-piperazinyl]ethyl]-, dihydrochloride (9CI) (CA INDEX NAME)

●2 HCl

RN 216674-43-0 CAPLUS

CN 2(1H)-Quinolinone, 7-fluoro-4-[2-[4-(6-fluoro-1-methyl-1H-indazol-3-yl)-1-piperazinyl]ethyl]-, dihydrochloride (9CI) (CA INDEX NAME)

•2 HCl

RN 216674-49-6 CAPLUS

CN 1(2H)-Quinolineacetamide, 7-fluoro-4-[2-[4-(6-fluoro-1-methyl-1H-indazol-3-yl)-1-piperazinyl]ethyl]-2-oxo-, dihydrochloride (9CI) (CA INDEX NAME)

●2 HCl

RN 216674-53-2 CAPLUS

CN 2(1H)-Quinolinone, 7-fluoro-4-[2-[4-(6-fluoro-1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]-, dihydrochloride (9CI) (CA INDEX NAME)

•2 HCl

L10 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1995:682542 CAPLUS

DN 123:83356

TI Preparation of 3-(1-piperazinyl)-1,2-benzisothiazole derivatives with antipsychotic effect

IN Fukuda, Yoshimasa; Sasaki, Toshiro; Nakatani, Yuuko; Ichimaru, Yasuyuki; Imanishi, Taiichiro

PA Meiji Seika K. K., Japan

SO PCT Int. Appl., 95 pp.

CODEN: PIXXD2

DT Patent LA Japanese FAN.CNT 1

	PATENT NO.					KIND DATE			APPLICATION NO.							DATE			
ΡI	WO 9418197			A1 19940818				WO 1	994-	JP15	9		19940203						
		W:	CN,	JP,	KR,	US													
		RW:	ΑT,	BE,	CH,	DE,	DK.	, ES,	FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE	
	EP 635506			A 1		1995	0125		EP 1	994-	9058	41		1	9940	203			
		R:	AT,	BE,	CH,	DE,	DK	, ES,	FR,	GB,	IT,	LI,	NL,	SE					
	CN 1102524					7		1005	0607		CNI 1	004	1000	12		1	0040	202	

CN 1103534 A 19950607 CN 1994-190042 19940203 CN 1050604 B 20000322

US 5599815 A 19970204 US 1994-318857 19941220 PRAI JP 1993-17505 A 19930204 WO 1994-JP1 A 19940104

19940203

WO 1994-JP159 W
OS MARPAT 123:83356

GΙ

$$N (CH_2)_n W$$

AB Compds. represented by general formula [I; n = 2-4; W = heterocyclyl, e.g., Q - Q2; m = 0-2; A = CH2, CH, N, NH; B = CH2, CH, N, NH, S; provided that both A and B .noteq. N or NH; X = CH, N, S, bond; Y = CH, N; R1 = H, halo, lower (halo)alkyl, (un)substituted Ph, OH, NO2, lower alkoxy, NH2, cyano; R2, R3 = H, halo, lower (halo)alkyl or alkoxy, NH2, cyano, provided that when X = bond, R2 is not present; or R2R3 = (CH2)p (wherein p = 3-5)] and pharmacol. acceptable salts thereof, reduced in the adverse effect against the extrapyramidal system and hence useful as an antipsychotic agent with few side effects, are prepd. Thus, 0.29 g 2-hydroxyquinoline was dissolved in DMF and treated with 80 mg NaH at 60.degree. for 30 min with stirring followed by cooling the reaction mixt. to room temp. and adding 2.16 g 1,4-dibromobutane and the resulting mixt. was stirred at 60.degree. for 4 h to give 64% 1-(4-bromobutyl)-2(1H)-quinolinone (II). II 0.56, 3-(1-piperazinyl)-1,2-benzisothiazole 0.44, and K2CO3 0.33 g were suspended in DMF and stirred at room temp. for 12 h to give 80% title

ΙT

CN

compd. I (n = 4, W = 2-oxo-1, 2-dihydro-1-quinolinyl). II (n = 4, W = 9-carbazolyl) and II (n = 3, W = 2-oxo-1, 2-dihydro-1-quinolinyl) showed ED50 of 1.15 and 0.92 mg/kg i.p., resp., for inhibiting methamphetamine-induced spontaneous movement of mice (vs. 0.16 and 1.05 mg/kg i.p. for haloperidol and chlorpromazine, resp.) and induced catalepsy in mice at ED50 of >100 and 83.3 mg/kg i.p. in mice (vs. 1.3 and 6.2 mg/kg i.p. for haloperidol and chlorpromazine, resp.).

165109-31-9P 165109-35-3P 165109-39-7P 165109-40-0P 165109-54-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of [N-(heterocyclylalkyl)piperazinyl] benzisothiazole derivs. as antipsychotics)

RN 165109-31-9 CAPLUS

2(1H)-Quinolinone, 1-[4-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]butyl]-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 165109-35-3 CAPLUS

CN 2(1H)-Quinolinone, 1-[3-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)

10/460752

● HCl

RN 165109-39-7 CAPLUS

CN 6(5H)-Phenanthridinone, 5-[4-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]butyl]-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 165109-40-0 CAPLUS

CN Phenanthridine, 6-[4-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]butoxy]-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 165109-54-6 CAPLUS

CN 2(1H)-Quinolinone, 1-[4-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]butyl]-3,4-dihydro-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

L10 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1995:657604 CAPLUS

DN 123:55870

TI Preparation of indazole derivatives as antipsychotics

IN Sasaki, Toshiro; Nakatani, Juko; Hiranuma, Toyoichi; Kashima, Hiroko; Fukuda, Yoshimasa

PA Meiji Seika Co, Japan

SO Jpn. Kokai Tokkyo Koho, 23 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

212110111 1				
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 07033744	A2	19950203	JP 1993-204612	19930727
PRAI JP 1993-204612		19930727		

OS MARPAT 123:55870

GΙ

$$V = \begin{bmatrix} N & N(CH_2)_nW \\ N & N \end{bmatrix}$$

AB The title compds. I [n = 2 - 6; V = H, halo; R1 = H, alkyl, etc.; W = heterocycle (further details on said heterocycle are given)] are prepd. Indazole deriv. II (prepn. given) showed ED50 of 0.50 mg/Kg i.p. against methamphetamine-induced activities in mice, vs. ED50 of 0.16 mg/Kg i.p. shown by haloperidol. In a test for catalepsy-causing activity in mice, II showed ED50 of 18 mg/Kg i.p., vs. ED50 of 1.3 mg/Kg i.p. shown by haloperidol.

IT 164519-46-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

II

(prepn. of indazole derivs. as antipsychotics)

RN 164519-46-4 CAPLUS

CN 6(5H)-Phenanthridinone, 5-[4-[4-(1H-indazol-3-yl)-1-piperazinyl]butyl]-(9CI) (CA INDEX NAME)

IT 164519-94-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

10/460752

L10 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN AN 1991:492295 CAPLUS

DN 115:92295

TI Preparation of heteroarylpiperazines as antipsychotic agents

IN Howard, Harry R.

PA Pfizer Inc., USA

SO Eur. Pat. Appl., 20 pp.

CODEN: EPXXDW

DT Patent

LA English

FAN.CNT 1

PAN.	~IVT	1																
	PAT	CENT	NO.			KIND		DATE			API	LICAT	CION	NO.		DATE		
ΡI	EP 409435					A1		19910123			ΕP	1990-		19900629				
	ΕP	4094	35			В1		19941026										
		R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GF	R, IT,	LI,	LU,	NL,	SE	ı	
	WO	9100	863			A1		1991	0124		WO	1989-	-US29	954			19890707	
		W:	FI,	HU,	NO,	RO,	SU,	, US										
	ES	2062	374			Т3		1994	1216		ES	1990-	-3071	166			19900629	
	JP	0304	4388			A2		1991	0226		JΡ	1990-	-1761	L20			19900703	
	JP	0701	7633			B4		1995	0301									
	CA	2020	611			AA		1991	0108		CA	1990-	-2020	611			19900706	
	US	5350	747			Α		1994	0927		US	1992-	-8360	19			19920220	
PRAI	WO	1989	-US29	954		Α		1989	0707									
os	MAI	RPAT	115:	9229	5													
GI																		

$$R^{1}N$$
 $NZCH_{2}$
 N^{1}
 N^{2}
 N^{1}
 N^{2}
 N^{1}
 N^{2}
 N^{2}
 N^{3}
 N^{4}
 N^{1}
 N^{2}
 N^{4}
 N^{4}

AΒ The title compds. [I; W1 = CR2R3; W2 = CR4R5; W3 = CR6R7; 1 of W1-W3 may be absent; R1 = (substituted) benzisoxazolyl, benzisothiazolyl, benzopyrazolyl; R2-R7 = H, alkyl, 2 of them may form alkylene, alkenylene; X1 = H, halo, C1-4 alkyl, alkoxy, NO2, cyano, etc.; Y1 = H, C1-4 alkyl, (substituted) Ph, etc.; X1Y1 = heterocyclyl; Z = C1-6 alkylene], useful as antipsychotic agents (no data), were prepd. A mixt. of piperazine deriv. II, quinolinone III (prepn. given), Na2CO3, and KI in MIBK was heated at 90.degree. under N to give 13% title compd. IV, sepd. as HCl.1/2 H2O. Also prepd. were 17 addnl. I and numerous intermediates.

IT 133999-10-7P 134017-19-9P 134017-20-2P 134017-21-3P 134017-22-4P 134017-23-5P 134017-24-6P 134017-25-7P 134017-26-8P 134017-27-9P 134017-28-0P 134017-29-1P 134017-30-4P 134017-31-5P 134017-32-6P 135357-15-2P 135357-16-3P RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of, as antipsychotic agent)

RN133999-10-7 CAPLUS

CN 2(1H)-Quinolinone, 7-chloro-3,4-dihydro-6-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]-4,4-dimethyl- (9CI) (CA INDEX NAME)

10/460752

RN 134017-19-9 CAPLUS

CN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]-3,4-dihydro-, monohydrochloride (9CI) (CA INDEX NAME)

HCl

RN 134017-20-2 CAPLUS

CN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]-1-ethyl-3,4-dihydro- (9CI) (CA INDEX NAME)

RN 134017-21-3 CAPLUS

CN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]-3,4-dihydro-4-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ &$$

RN 134017-22-4 CAPLUS

CN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]-3,4-dihydro-3-methyl- (9CI) (CA INDEX NAME)

RN 134017-23-5 CAPLUS

10/460752

CN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]-3,4-dihydro-7-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ &$$

RN 134017-24-6 CAPLUS

CN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]-3,4-dihydro-3,3-dimethyl- (9CI) (CA INDEX NAME)

RN 134017-25-7 CAPLUS

CN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]-3,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)

RN 134017-26-8 CAPLUS

CN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]-3,4-dihydro-4,7-dimethyl- (9CI) (CA INDEX NAME)

RN 134017-27-9 CAPLUS

CN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]-

3,4-dihydro-1,4-dimethyl- (9CI) (CA INDEX NAME)

RN 134017-28-0 CAPLUS

CN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]-3,4-dihydro-1,3,3-trimethyl- (9CI) (CA INDEX NAME)

RN 134017-29-1 CAPLUS

CN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]-3,4-dihydro-4,4,7-trimethyl- (9CI) (CA INDEX NAME)

RN 134017-30-4 CAPLUS

CN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]-7-chloro-3,4-dihydro- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ &$$

RN 134017-31-5 CAPLUS

CN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]-7-chloro-1-ethyl-3,4-dihydro-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \text{Et} \\ & & & \\ & & & \\ & &$$

RN 134017-32-6 CAPLUS

CN 2(1H)-Quinolinone, 6-[3-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]propyl]-3,4-dihydro-4-methyl- (9CI) (CA INDEX NAME)

RN 135357-15-2 CAPLUS

CN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]-3,4-dihydro-4-methyl-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 135357-16-3 CAPLUS

CN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]-3,4-dihydro-4-methyl-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

=> file caold		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	67.82	601.67
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-9.49	-38.69

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=> s 19 L11 0 L9

=> file caplus COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 1.29 602.96 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE 0.00 -38.69

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s US2003-660908/APPS

1 US2003-660908/AP

0 US2003-660908/PRN

L12

1 US2003-660908/APPS

(US2003-660908/AP, PRN)

=> file reg

COST IN U.S. DOLLARS

SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL

CA SUBSCRIBER PRICE ENTRY SESSION 0.00 -38.69

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STRUCTURE FILE UPDATES: 16 SEP 2005 HIGHEST RN 863378-74-9 DICTIONARY FILE UPDATES: 16 SEP 2005 HIGHEST RN 863378-74-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

* The CA roles and document type information have been removed from * the IDE default display format and the ED field has been added, * effective March 20, 2005. A new display format, IDERL, is now * available and contains the CA role and document type information. * *

Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=> tra 112 RN

L13 TRANSFER L12 1- RN : 350 TERMS

L14 350 L13

=> s 114 and piperazine/cn

1 PIPERAZINE/CN

L15 1 L14 AND PIPERAZINE/CN

=> d scan 114

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN Glycine, N-[3-[[4-[3-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]propyl]phenyl]amino]-3-oxopropyl]-N-methyl-, ethyl ester (9CI)

MF C28 H37 N5 O3 S

PAGE 1-B

PAGE 1-A

- OEt

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN IN 1,4,7-Trioxaspiro[4.4]nonane-9-carboxamide, N-[4-[2-[4-(1,2-benzisothiazol-

3-y1)-1-piperazinyl]ethyl]-2-methylphenyl]- (9CI) MF C27 H32 N4 O4 S

PAGE 1-A

PAGE 2-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[2-[4-(7-fluoro-1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]-3,4-dimethyl- (9CI)

MF C24 H25 F N4 O S

$$\begin{array}{c|c} F & H & O \\ \hline & N & N & CH_2 - CH_2 \\ \hline & Me & Me \\ \end{array}$$

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]1-(2,2-dimethylpropyl)-3,4-dihydro-4,4,8-trimethyl- (9CI)

MF C30 H40 N4 O S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisoxazol-3-yl)-1-piperazinyl]ethyl]-1(3,3-dimethyl-2-oxobutyl)-3,4-dimethyl- (9CI)

MF C30 H36 N4 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisoxazol-3-yl)-1-piperazinyl]ethyl]3,4-dihydro-4-methyl-1-(2-methylpropyl)- (9CI)

MF C27 H34 N4 O2

$$\begin{array}{c|c} & i-Bu \\ \hline & N \\ \hline & N \\ \hline & N \\ \hline & N \\ \hline & Me \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]1-ethyl-3,4-dihydro-4-methyl- (9CI)

MF C25 H30 N4 O S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]3,4-dihydro-1-(methoxymethyl)-3,3-dimethyl- (9CI)

MF C26 H32 N4 O2 S

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 1(2H)-Quinolineacetamide, 6-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]-3,4-dihydro-.alpha.,3-dimethyl-2-oxo-N-phenyl- (9CI)

MF C32 H35 N5 O2 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]4-propyl- (9CI)
MF C25 H28 N4 O S

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN 2(1H)-Quinolinone, 6-(3-chloropropyl)-3,4-dihydro-4,4,8-trimethyl- (9CI)
MF C15 H20 C1 N O

$$C1-(CH_2)_3$$
Me
Me
Me
Me

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN Quinoline, 1-acetyl-6-(3-chloropropyl)-1,2,3,4-tetrahydro-3,3-dimethyl(9CI)
MF C16 H22 C1 N O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[3-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]propyl]7-fluoro-3,4-dihydro-1,4,4-trimethyl- (9CI)

MF C26 H31 F N4 O S

CI COM

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 3,4-dihydro-6-[3-[4-(1H-indazol-3-yl)-1-piperazinyl]propyl]-3-methyl- (9CI)

MF C24 H29 N5 O

$$\begin{array}{c|c}
H \\
N \\
N \\
N \\
N \\
Me
\end{array}$$

$$\begin{array}{c}
H \\
N \\
N \\
Me
\end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[3-[4-(1,2-benzisoxazol-3-yl)-1-piperazinyl]propyl]3,4-dihydro-4-methyl- (9CI)

MF C24 H28 N4 O2

$$O$$
 N
 N
 N
 N
 N
 M
 M
 M

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[2-[4-(6-fluorobenzo[b]thien-3-yl)-1-piperazinyl]ethyl]-3,4-dihydro-4-methyl-, (4S)- (9CI)

MF C24 H26 F N3 O S

Absolute stereochemistry. Rotation (-).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN IN 1,2-Benzisoxazole, 6-methyl-3-(1-piperazinyl)- (9CI) MF C12 H15 N3 O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN IN 1,2-Benzisothiazole, 5-methoxy-3-(1-piperaziny1)- (9CI) MF C12 H15 N3 O S CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

Page 45

IN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]8-ethyl-3,4-dihydro-4,4-dimethyl- (9CI)
MF C26 H32 N4 O S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]-7-chloro-3,4-dihydro-4,4,8-trimethyl- (9CI)

MF C25 H29 C1 N4 O S

CI COM

$$\begin{array}{c|c} & & & \\ & & & \\$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 3,4-dihydro-6-[2-[4-(1H-indazol-3-yl)-1-piperazinyl]ethyl]-4,4-dimethyl- (9CI)

MF C24 H29 N5 O

$$\begin{array}{c|c} H & H & N \\ \hline N & N & CH_2-CH_2 \\ \hline & Me & Me \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN 2(1H)-Quinolinone, 6-(chloroacetyl)-3,4-dihydro-3,4-dimethyl- (9CI)
MF C13 H14 C1 N O2

$$\begin{array}{c|c} & & & H & O \\ \hline \text{ClCH}_2 - C & & & Me \\ \hline & & & Me \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisoxazol-3-yl)-1-piperazinyl]ethyl]3,4-dihydro-1,4-dimethyl- (9CI)

MF C24 H28 N4 O2

CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN IN 1,2-Benzisothiazole, 3-(1-piperazinyl)-, hydrochloride (9CI) MF C11 H13 N3 S . x Cl H

●x HCl

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN 2(1H)-Quinolinone, 6-(2-chloroethyl)-3,4-dihydro-4,4-dimethyl- (9CI)
MF C13 H16 Cl N O

$$C1CH_2-CH_2$$
Me Me

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN IN 2-Butenamide, 3-methyl-N-(2-methylphenyl)- (9CI) MF C12 H15 N O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN IN 1,2-Benzisoxazole, 6-fluoro-3-(4-piperidinyl)- (9CI) MF C12 H13 F N2 O CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN IN 1H-Indazole, 3-chloro- (6CI, 8CI, 9CI) MF C7 H5 Cl N2

CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN Cyclohexanecarboxylic acid, 2-oxo-, ethyl ester (6CI, 7CI, 8CI, 9CI)

MF C9 H14 O3

CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN Butanoic acid, 4,4,4-trifluoro-3-oxo-, ethyl ester (9CI)

MF C6 H7 F3 O3

CI COM

$$\begin{array}{c|c} & \text{O} & \text{O} \\ \parallel & \parallel \\ \text{F}_3\text{C}-\text{C}-\text{CH}_2-\text{C}-\text{OEt} \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):30

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisoxazol-3-yl)-1-piperazinyl]ethyl]3,4-dihydro-1,4,4-trimethyl- (9CI)

MF C25 H30 N4 O2

CI COM

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 4H-Pyrrolo[3,4-c]quinolin-4-one, 8-[3-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]propyl]-1,2,3,5-tetrahydro-2-methyl- (9CI)

MF C26 H29 N5 O S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 1,4,7-Trioxaspiro[4.4]nonane-9-carboxylic acid, ethyl ester (9CI)

MF C9 H14 O5

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[2-[4-(5-chloro-1,2-benzisoxazol-3-yl)-1-piperazinyl]ethyl]-3,4-dimethyl- (9CI)

MF C24 H25 Cl N4 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]1-(2-ethylbutyl)-3,4-dihydro-4,4,8-trimethyl- (9CI)

MF C31 H42 N4 O S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 1(2H)-Quinolineacetic acid, 6-[2-[4-(1,2-benzisoxazol-3-yl)-1-piperazinyl]ethyl]-3,4-dimethyl-2-oxo-, ethyl ester (9CI)

MF C28 H32 N4 O4

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 1(2H)-Quinolineacetonitrile, 6-[2-[4-(1,2-benzisoxazol-3-yl)-1-piperazinyl]ethyl]-3,4-dihydro-.alpha.,4-dimethyl-2-oxo- (9CI)

MF C26 H29 N5 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]-3,4-dihydro-4-methyl-1-(2-oxo-2-phenylethyl)- (9CI)

MF C31 H32 N4 O2 S

$$\begin{array}{c|c} & & & \\ &$$

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]-1-(3,3-dimethyl-2-oxobutyl)-3,4-dihydro-3,3-dimethyl- (9CI)

MF C30 H38 N4 O2 S

$$\begin{array}{c|c} & \circ & \\ & \vdash & \\ \text{CH}_2-\text{C}-\text{Bu-t} \\ & & \\$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 1(2H)-Quinolineacetamide, 6-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]-3,4-dihydro-3-methyl-2-oxo-(9CI)

MF C25 H29 N5 O2 S

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & &$$

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN 1H,5H-Benzo[ij]quinolizin-5-one, 2,3,6,7-tetrahydro-7,7-dimethyl- (9CI)
MF C14 H17 N O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN 4H-Cyclopenta[c]quinolin-4-one, 8-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]-1,2,3,5-tetrahydro- (9CI)
MF C25 H26 N4 O S

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[3-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]propyl]3,4-dihydro-4,4,8-trimethyl- (9CI)

MF C26 H32 N4 O S

$$\begin{array}{c|c} & \text{Me} & \text{H} \\ & \text{N} & \text{N} \\ & \text{N} & \text{N} \\ & \text{Me} & \text{Me} \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN Quinoline, 1-acetyl-6-[3-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]propyl]-1,2,3,4-tetrahydro-3,3-dimethyl- (9CI)

MF C27 H34 N4 O S

CI COM

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN 2(1H)-Quinolinone, 7-fluoro-3,4-dihydro-4,4-dimethyl- (9CI)
MF C11 H12 F N O

$$\begin{array}{c|c} F & H & O \\ \hline & Me & Me \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN 2(1H)-Quinolinone, 6-(3-chloropropyl)-3,4-dihydro-3-methyl- (9CI)
MF C13 H16 C1 N O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN 2(1H)-Quinolinone, 7-chloro-6-(3-chloropropyl)-3,4-dihydro-4,4-dimethyl(9CI)
MF C14 H17 C12 N O

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN Piperazine, 1-benzo[b]thien-3-yl-, monohydrochloride (9CI)
MF C12 H14 N2 S . C1 H

● HCl

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN IN 1,2-Benzisothiazole, 7-fluoro-3-(1-piperaziny1)- (9CI) MF C11 H12 F N3 S CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisoxazol-3-yl)-1-piperazinyl]ethyl]3,4-dihydro-4,4,8-trimethyl- (9CI)

MF C25 H30 N4 O2

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]7-fluoro-3,4-dihydro-4,4,8-trimethyl- (9CI)

MF C25 H29 F N4 O S

CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN 2(1H)-Quinolinone, 6-(2-chloroethyl)-3,4-dihydro-4,4,8-trimethyl- (9CI)
MF C14 H18 C1 N O

$$C1CH_2-CH_2$$
Me
Me
Me
Me

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN IN 2(1H)-Quinolinone, 3,4-dihydro-6-[2-[4-(1H-indazol-3-yl)-1-

piperazinyl]ethyl]-4-methyl- (9CI)

MF C23 H27 N5 O

$$\begin{array}{c|c}
H \\
N \\
N \\
N \\
N \\
Me
\end{array}$$

$$\begin{array}{c}
H \\
N \\
N \\
Me$$

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN IN 2(1H)-Quinolinone, 6-(2-chloroethyl)-3,4-dimethyl- (9CI) MF C13 H14 Cl N O

$$C1CH_2-CH_2$$
 Me
 Me

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisoxazol-3-yl)-1-piperazinyl]ethyl]3,4-dihydro-1,4-dimethyl-, hydrochloride (10:11) (9CI)

MF C24 H28 N4 O2 . 11/10 C1 H

$$\begin{array}{c|c}
 & Me \\
 & N \\
 & N \\
 & N \\
 & N \\
 & Me
\end{array}$$

●11/10 HCl

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN 2(1H)-Quinolinone, 6-(2-chloroethyl)-3,4-dihydro-4-methyl-, (4S)- (9CI)
MF C12 H14 Cl N O

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN 2(1H)-Quinolinone, 6-(2-chloroethyl)-3,4-dihydro-3-methyl- (9CI)
MF C12 H14 Cl N O

$$\begin{array}{c|c} & & H & O \\ \hline & & N & \\ \hline & & C1CH_2-CH_2 & & Me \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN IN 1,2-Benzisoxazole, 5-chloro-3-(1-piperazinyl)- (9CI) MF C11 H12 C1 N3 O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN IN 2(1H)-Quinolinone, 3,4-dihydro-4-methyl-, (4S)- (9CI) MF C10 H11 N O

Absolute stereochemistry. Rotation (-).

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN IN Benzene, 1-(2-chloroethyl)-4-nitro- (6CI, 7CI, 8CI, 9CI) MF C8 H8 Cl N O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):30

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN IN Quinoline, 1,2,3,4-tetrahydro- (8CI, 9CI) MF C9 H11 N CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN IN 2-Propenoic acid, ethyl ester (9CI) MF C5 H8 O2 CI COM

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN 4H-Cyclopenta[c]quinolin-4-one, 1,2,3,5-tetrahydro-8-hydroxy- (9CI)
MF C12 H11 N O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN Benzenamine, 4-[2-[4-(1,2-benzisoxazol-3-yl)-1-piperazinyl]ethyl]- (9CI)
MF C19 H22 N4 O

$$\begin{array}{c|c}
 & \text{N} & \text{N} & \text{CH}_2 - \text{CH}_2 \\
\hline
 & \text{N} & \text{N} & \text{N} & \text{CH}_2 - \text{CH}_2 \\
\hline
 & \text{N} & \text{N} & \text{N} & \text{N} & \text{N} & \text{CH}_2 \\
\hline
 & \text{N} \\
\hline
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 & \text{N} &$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN Furo[3,4-c]quinolin-4(1H)-one, 8-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]-3,5-dihydro-6-methyl- (9CI)

MF C25 H26 N4 O2 S

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[2-[4-(6-fluoro-1,2-benzisoxazol-3-yl)-1-piperazinyl]ethyl]-3,4-dimethyl- (9CI)

MF C24 H25 F N4 O2

$$\begin{array}{c|c} F & O & N & N - CH_2 - CH_2 \\ \hline & N & Me \\ \hline \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]3,4-dihydro-4,4,8-trimethyl-1-pentyl- (9CI)

MF C30 H40 N4 O S

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 1(2H)-Quinolineacetamide, 6-[2-[4-(1,2-benzisoxazol-3-yl)-1-piperazinyl]ethyl]-3,4-dimethyl-2-oxo-(9CI)

MF C26 H29 N5 O3

$$\begin{array}{c|c}
 & O \\
 & CH_2-C-NH_2 \\
\hline
 & N \\
 & N \\
\hline
 & N \\
 & Me \\
 & Me \\
\end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisoxazol-3-yl)-1-piperazinyl]ethyl]-1-(3,3-dimethyl-2-oxobutyl)-3,4-dihydro-4-methyl-(9CI)

MF C29 H36 N4 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 1(2H)-Quinolineacetic acid, 6-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]-3,4-dihydro-4-methyl-2-oxo-, ethyl ester (9CI)

MF C27 H32 N4 O3 S

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ &$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 1(2H)-Quinolineacetamide, 6-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]-3,4-dihydro-3,3-dimethyl-2-oxo- (9CI)

MF C26 H31 N5 O2 S

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & &$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[2-[4-(6-fluoro-1,2-benzisothiazol-3-yl)-1piperidinyl]ethyl]-3,4-dihydro-4-methyl-, monohydrochloride, (4S)- (9CI)

MF C24 H26 F N3 O S . Cl H

Absolute stereochemistry.

HCl

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 1H,5H-Benzo[ij]quinolizin-5-one, 9-(2-chloroethyl)-2,3,6,7-tetrahydro(9CT)

MF C14 H16 Cl N O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]-3,4-dimethyl- (9CI)

MF C24 H26 N4 O S

$$\begin{array}{c|c} S & N & N - CH_2 - CH_2 \\ \hline & Me \end{array}$$

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 8-chloro-6-(3-chloropropyl)-3,4-dihydro-4,4-dimethyl(9CI)

MF C14 H17 C12 N O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN Quinoline, 6-(3-chloropropyl)-1,2,3,4-tetrahydro-4,4-dimethyl- (9CI)

MF C14 H20 C1 N

$$C1-(CH_2)$$
 3 Me Me

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[3-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]propyl]-7-fluoro-3,4-dihydro-4,4-dimethyl- (9CI)

Me

Me

MF C25 H29 F N4 O S

$$\begin{array}{c|c} & & & & \\ & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[3-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]propyl]3,4-dihydro-3-methyl- (9CI)

MF C24 H28 N4 O S

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ &$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[3-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]propyl]7-chloro-3,4-dihydro-4,4-dimethyl- (9CI)

MF C25 H29 Cl N4 O S

$$\begin{array}{c|c}
\text{C1} & \text{H} & \text{N} \\
\text{N} & \text{N} & \text{CH2} \\
\text{Me} & \text{Me} & \text{Me}
\end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 1-(2-ethoxyethyl)-6-[2-[4-(5-fluoro-1,2-benzisothiazol3-yl)-1-piperazinyl]ethyl]-3,4-dihydro-4,4,8-trimethyl-, monohydrochloride
(9CI)

MF C29 H37 F N4 O2 S . C1 H

HCl

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[2-[4-(5-chloro-1,2-benzisoxazol-3-yl)-1-piperazinyl]ethyl]-3,4-dihydro-4,4,8-trimethyl- (9CI)

MF C25 H29 C1 N4 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 8-chloro-6-(2-chloroethyl)-3,4-dihydro-4,4-dimethyl(9CI)

MF C13 H15 C12 N O

$$C1$$
 H
 N
 O
 $C1CH_2-CH_2$
 Me
 Me

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-(chloroacetyl)-7-fluoro-3,4-dihydro-4,4,8-trimethyl(9CI)

MF C14 H15 C1 F N O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]3,4-dihydro-4,4,8-trimethyl- (9CI)

MF C25 H30 N4 O S

CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN IN 2(1H)-Quinolinone, 3,4-dihydro-3,3,4-trimethyl- (9CI) MF C12 H15 N O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisoxazol-3-yl)-1-piperazinyl]ethyl]3,4-dimethyl-, monohydrochloride (9CI)
MF C24 H26 N4 O2 . Cl H

$$\begin{array}{c|c}
 & \text{N} & \text{N} & \text{CH}_2 - \text{CH}_2
\end{array}$$

● HCl

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisoxazol-3-yl)-1-piperazinyl]ethyl]3,4-dihydro-4-methyl-, (4S)- (9CI)

MF C23 H26 N4 O2

Absolute stereochemistry. Rotation (+).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[3-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]propyl]3,4-dihydro-4-methyl- (9CI)

MF C24 H28 N4 O S

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN 2(1H)-Quinolinone, 6-(3-chloro-1-oxopropyl)-3,4-dihydro-4-methyl- (9CI)
MF C13 H14 Cl N O2

$$C1CH_2-CH_2-C$$

$$O$$

$$Me$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN IN 2(1H)-Quinolinone, 3,4-dihydro-3,3-dimethyl- (9CI) MF C11 H13 N O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):30

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN IN 2(1H)-Quinolinone, 3,4-dihydro-4,4-dimethyl- (9CI) MF C11 H13 N O

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN Quinoline, 1,2,3,4-tetrahydro-1-(3-methyl-1-oxo-2-butenyl)- (9CI)
MF C14 H17 N O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN Benzene, (2-chloroethyl) - (7CI, 8CI, 9CI)

MF C8 H9 Cl

CI COM

 $ClCH_2-CH_2-Ph$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN Propane, 1,3-dibromo- (8CI, 9CI)

MF C3 H6 Br2

CI COM

 $Br-CH_2-CH_2-CH_2-Br$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 4H-Cyclopenta[c]quinolin-4-one, 8-[3-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]propoxy]-1,2,3,5-tetrahydro- (9CI)

MF C26 H28 N4 O2 S

CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN Furo[3,4-c]quinolin-4(1H)-one, 8-[2-[4-(1,2-benzisoxazol-3-yl)-1-piperazinyl]ethyl]-3,5-dihydro- (9CI)

MF C24 H24 N4 O3

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[2-[4-(6-fluoro-1,2-benzisoxazol-3-yl)-1-piperidinyl]ethyl]-3,4-dimethyl- (9CI)

MF C25 H26 F N3 O2

$$\begin{array}{c|c} F & & \\ \hline \\ N & \\ \hline \\ N & \\ \end{array} \begin{array}{c} N \\ \hline \\ CH_2 - CH_2 \end{array} \begin{array}{c} H \\ N \\ \hline \\ Me \end{array} \begin{array}{c} O \\ \\ Me \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]1-cyclobutyl-3,4-dihydro-4,4,8-trimethyl- (9CI)

MF C29 H36 N4 O S

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisoxazol-3-yl)-1-piperazinyl]ethyl]3,4-dimethyl-1-(2,2,2-trifluoroethyl)- (9CI)

MF C26 H27 F3 N4 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]3,4-dimethyl-1-(2,2,2-trifluoroethyl)- (9CI)

MF C26 H27 F3 N4 O S

$$\begin{array}{c|c} & \text{CH}_2\text{--}\text{CF}_3 \\ \hline & \text{N} & \text{N} & \text{CH}_2\text{--}\text{CH}_2 \\ \hline & \text{Me} \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN IN 1(2H)-Quinolineacetamide, 6-[2-[4-(1,2-benzisoxazol-3-yl)-1-

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 1(2H)-Quinolineacetamide, 6-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]-3,4-dihydro-.alpha.,4-dimethyl-2-oxo- (9CI)

MF C26 H31 N5 O2 S

$$\begin{array}{c|c} & \text{Me} & \text{O} \\ & \text{II} \\ \text{CH-C-NH2} \\ \\ & \text{N} \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 1(2H)-Quinolineacetonitrile, 6-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]-3,4-dihydro-.alpha.,3-dimethyl-2-oxo- (9CI)

MF C26 H29 N5 O S

$$\begin{array}{c|c} & \text{CN} \\ & \text{CH-Me} \\ & \\ & \text{N} \\ & \text{N} \\ & \text{N} \\ & \text{N} \\ & \text{Me} \\ \end{array}$$

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[2-[4-(6-fluoro-1,2-benzisoxazol-3-yl)-1-piperidinyl]ethyl]-3,4-dihydro-4-methyl-, (4S)- (9CI)

MF C24 H26 F N3 O2

Absolute stereochemistry. Rotation (-).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 1H,5H-Benzo[ij]quinolizin-5-one, 9-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]-2,3,6,7-tetrahydro- (9CI)

MF C25 H28 N4 O S

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[3-[4-(1,2-benzisoxazol-3-yl)-1-piperazinyl]propyl]-8-ethyl-3,4-dihydro-4,4-dimethyl- (9CI)

MF C27 H34 N4 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[3-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]propyl]8-chloro-3,4-dihydro-4,4-dimethyl- (9CI)

MF C25 H29 C1 N4 O S

$$\begin{array}{c|c}
 & C1 & H & N & C1 \\
 & N & N & (CH_2)_3 & Me & Me
\end{array}$$

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN Quinoline, 1-acetyl-6-(3-chloropropyl)-7-fluoro-1,2,3,4-tetrahydro-4,4dimethyl- (9CI)

MF C16 H21 C1 F N O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[3-[4-(1,2-benzisoxazol-3-yl)-1-piperazinyl]propyl]3,4-dihydro-4-methyl-, (4R)- (9CI)

MF C24 H28 N4 O2

Absolute stereochemistry.

$$(CH_2)_3$$
 H
 N
 R
 Me

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[3-[4-(1,2-benzisoxazol-3-yl)-1-piperazinyl]propyl]3,4-dihydro-3,3-dimethyl- (9CI)
MF C25 H30 N4 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN 2(1H)-Quinolinone, 6-(3-chloropropyl)-3,4-dihydro-4,4-dimethyl- (9CI)
MF C14 H18 C1 N O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[2-[4-(5-fluoro-1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]-3,4-dihydro-4,4,8-trimethyl-1-(1-methylethyl)-,monohydrochloride (9CI)

MF C28 H35 F N4 O S . Cl H

● HCl

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN IN 1,2-Benzisoxazole, 5-fluoro-3-(1-piperazinyl)- (9CI)

MF C11 H12 F N3 O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN 2(1H)-Quinolinone, 8-chloro-3,4-dihydro-4,4-dimethyl- (9CI)
MF C11 H12 C1 N O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]7-fluoro-3,4-dihydro-4,4,8-trimethyl-, monohydrochloride (9CI)

MF C25 H29 F N4 O S . Cl H

HCl

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]3,4-dihydro-1,3,3,4,4-pentamethyl-, monohydrochloride (9CI)

MF C27 H34 N4 O S . Cl H

$$\begin{array}{c|c} & & & \\ & & & \\$$

● HCl

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisoxazol-3-yl)-1-piperazinyl]ethyl]3,4-dihydro-3,3,4-trimethyl- (9CI)

MF C25 H30 N4 O2

$$\begin{array}{c|c} & & & \\ &$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisoxazol-3-yl)-1-piperazinyl]ethyl]3,4-dihydro-3-methyl- (9CI)

MF C23 H26 N4 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN IN 1H-Indole, 2,3-dihydro-1-(3-methyl-1-oxo-2-butenyl)- (9CI) MF C13 H15 N O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 350 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 2(1H)-Quinolinone, 6-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]ethyl]3,4-dihydro-3-methyl- (9CI)

MF C23 H26 N4 O S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

=> d scan help

The following are valid formats:

Substance information can be displayed by requesting individual fields or predefined formats. The predefined substance formats are: (RN = CAS Registry Number)

REG - RN

SAM - Index Name, MF, and structure - no RN FIDE - All substance data, except sequence data

IDE - FIDE, but only 50 names SQIDE - IDE, plus sequence data

SQIDE3 - Same as SQIDE, but 3-letter amino acid codes are used

SQD - Protein sequence data, includes RN

SQD3 - Same as SQD, but 3-letter amino acid codes are used SQN - Protein sequence name information, includes RN

CALC - Table of calculated properties EPROP - Table of experimental properties

PROP - EPROP and CALC

Any CA File format may be combined with any substance format to obtain CA references citing the substance. The substance formats must be cited first. The CA File predefined formats are:

ABS -- Abstract

APPS -- Application and Priority Information

BIB -- CA Accession Number, plus Bibliographic Data

CAN -- CA Accession Number

CBIB -- CA Accession Number, plus Bibliographic Data (compressed)

IND -- Index Data

IPC -- International Patent Classification

PATS -- PI, SO

STD -- BIB, IPC, and NCL

IABS -- ABS, indented, with text labels

IBIB -- BIB, indented, with text labels

ISTD -- STD format, indented

OBIB ----- AN, plus Bibliographic Data (original)

OIBIB ----- OBIB, indented with text labels

SBIB ----- BIB, no citations SIBIB ----- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when it is available.

The MAX format is the same as ALL.

The IALL format is the same as ALL with BIB ABS and IND indented, with text labels.

For additional information, please consult the following help messages:

HELP DFIELDS -- To see a complete list of individual display fields. HELP FORMATS -- To see detailed descriptions of the predefined formats.

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IN Piperazine (8CI, 9CI)

MF C4 H10 N2

CI COM, RPS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> log h
COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)
SINCE FILE TOTAL
ENTRY SESSION
CA SUBSCRIBER PRICE

0.00 -38.69

SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 18:19:58 ON 18 SEP 2005